Bioaccumulation Model Check-In

CPG-EPA Conference Call

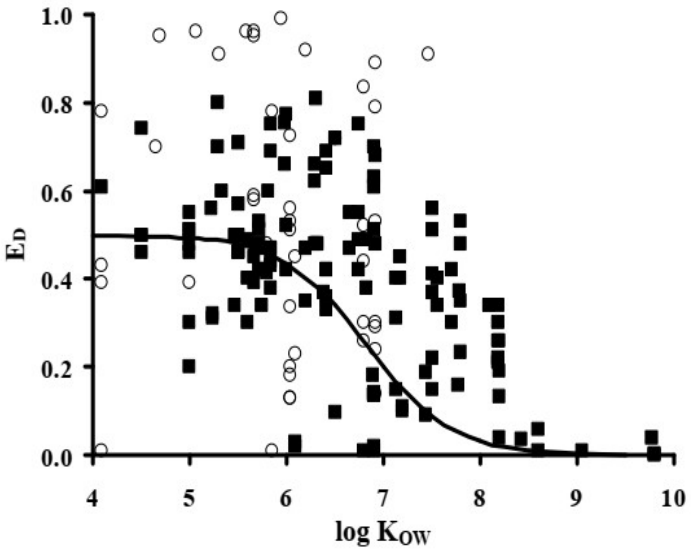
April 15, 2019

Agenda / Objectives

- Update on model calibration
  - E_D parameter research
  - Model parameterization notes
  - Discussion of alternate calibrations
- Next steps
  - Finalize current calibration
  - Model documentation
  - Schedule

E_D = Dietary chemical transfer efficiency Arnot and Gobas (2004)

- Empirical E_D observations = highly variable
  - Aquatic invertebrates = 0 to 100% (amphipods, mollusks, oligochaetes, snails, clams, bivalves)
  - Fish = 0 and 90%
- Possible explanations for variability in E_D:
  - differences in sorption coefficient of chemicals
  - composition of dietary matrices (e.g., organic carbon and soot carbon content)
  - digestibility of the dietary matrix
  - metabolic transformation
  - steric hindrance in gut membrane permeation
  - variability in food digestion between different species
- Large variability in the empirical data, but some trends:
  - Reduction in E_D with increasing K_{OW} for high-K_{OW} chemicals
  - Average E_D for chemicals with a log K_{OW} of 4 to 6 is ~50%



More about E_D Parameter: Additional Research

- General E_D trends:
  - Chlorination: More chlorination = lower E_D
  - Molecular volume: Higher MV = lower E_D
  - Molecular weight: No relationship
  - K_{OW}: Loose relationship
  - Species: No clear relationship
  - Diet type: Important factor to consider
- Two key conclusions:
  - E_D for dioxins/furans generally lower than E_D for PCBs
  - E_D expected to be lower for HpCDF than for TCDD

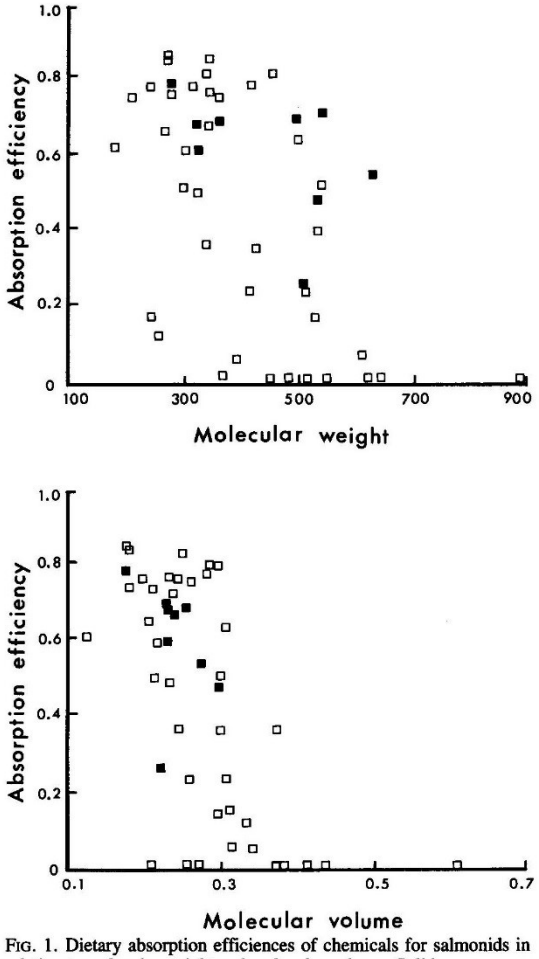


FIG. 1. Dietary absorption efficiences of chemicals for salmonids in relation to molecular weight and molecular volume. Solid squares represent some values observed for trout in this study reported in Table 1, and open squares represent the values for salmonids estimated from other studies in Table 2.

Source: Niimi and Oliver 1988

Distributions for E_D

- Use of different E_D values?
  - Some evidence to suggest that E_D values different
  - But insufficient evidence – would create more uncertainty (contrary to modeling fundamentals)

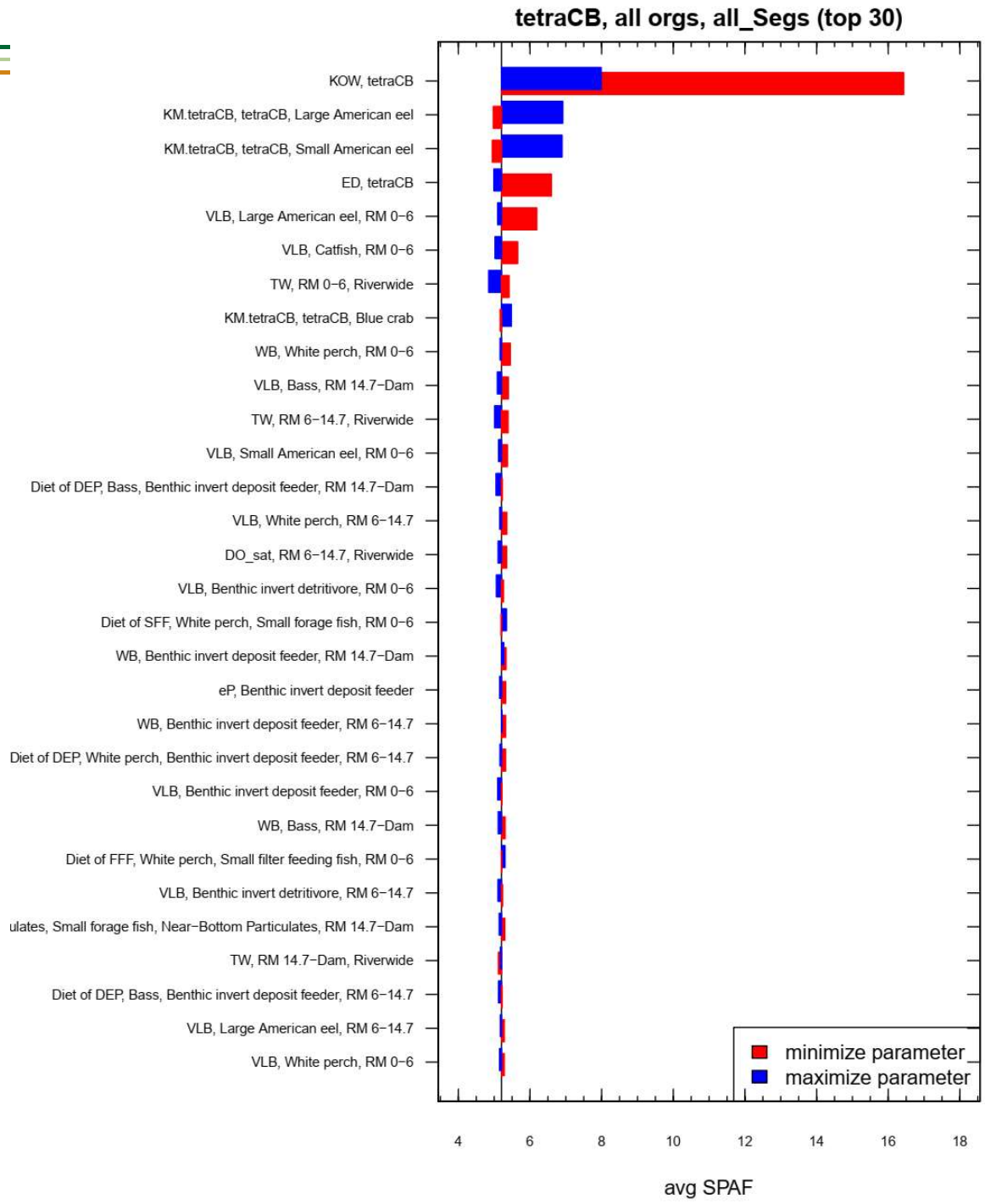
- Preliminary distributions based on research:

	E_D Values		
Chemical	**Nominal Value**	**Distribution Range (Literature)**	**Range Based on K_{OW} Equation**
2,3,7,8-TCDD	0.4	0.08 to 0.76	*0.004 to 0.48*
TetraCB	0.6	0.34 to 0.83	*0.30 to 0.48*
1,2,3,4,6,7,8-HpCDF	0.05	0 to 0.3	*0.002 to 0.11*

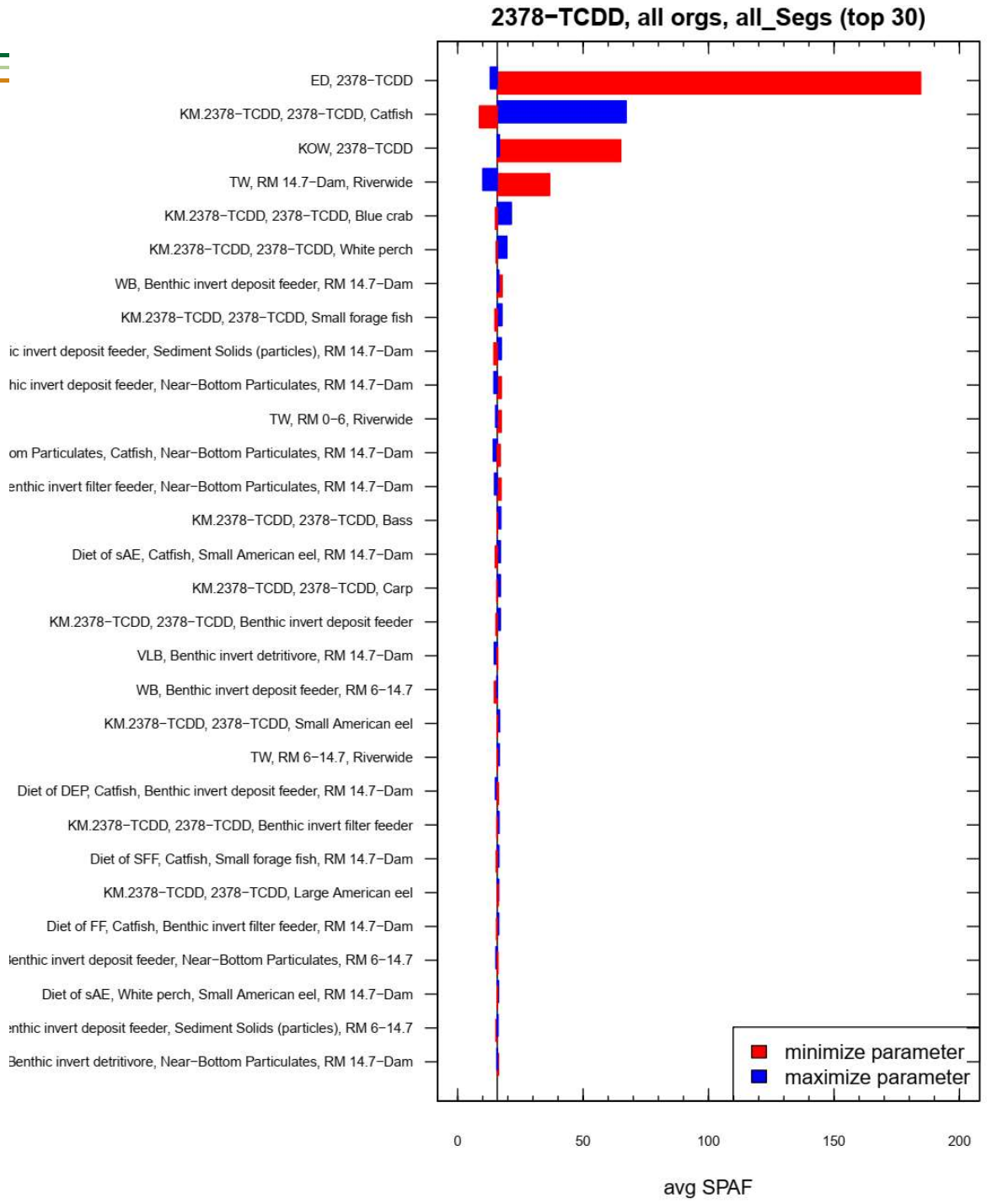
Model Calibration Update

- Calibration focusing on changes to the most sensitive parameters:
  - E_D (single vs. fish/inverts)?
  - Metabolic rate constants (K_M)
  - Select other parameters
  - Table of calibrated parameter values
- Review steady state and dynamic model output
  - Figures showing current calibration

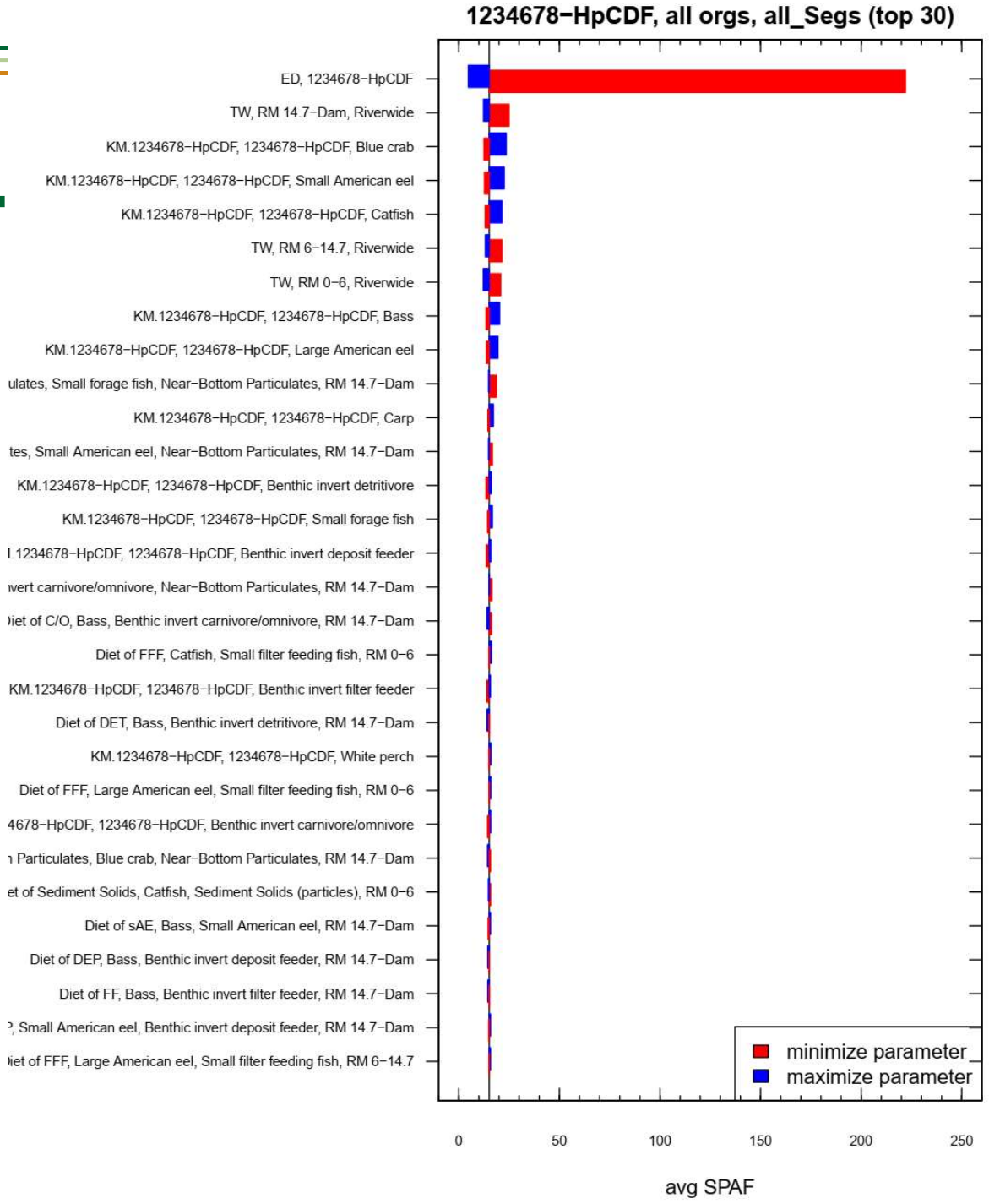
Tornado Plot: TetraCB



Tornado Plot: 2378-TCDD



Tornado Plot: 1234678-HpCDF



Current Calibration

	2378-TCDD			TetraCB			1234678-HpCDF		
Species	**RM 0-6**	**RM 6-14.7**	**RM 14.7-Dam**	**RM 0-6**	**RM 6-14.7**	**RM 14.7-Dam**	**RM 0-6**	**RM 6-14.7**	**RM 14.7-Dam**
DEP		21.7	8.6		5.4	6.5		16.2	4.6
FF									
DET									
C/O	11.5			5.7			8.0		
Small filter feeding fish		1.1			-1.4			1.0	
Small forage fish	1.1	3.4	-7.6	-1.6	-1.1	-1.6	2.3	-1.1	-1.4
Small American eel	-1.6	4.8	1.2	-2.9	1.2	1.0	-2.3	1.5	-1.5
Blue crab	-2.0	2.2	-22.7	-1.7	1.6	1.2	-2.9	-1.1	-2.1
Carp		-1.5	-6.7		-2.7	-1.6		-1.3	1.2
Catfish	-5.2	1.4	-47.1	-4.9	-1.2	-1.9	-2.8	2.4	1.2
White perch	-2.1	1.5	-11.1	-3.6	-1.8	-1.4	1.6	2.7	2.8
Large American eel	-1.1	1.6		-2.3	1.1		-1.7	-1.1	
Bass		-1.3	-5.1		-1.8	-3.7		1.4	-2.2
Average (all)	**2.2**	**2.1**	**14.5**	**2.8**	**1.5**	**1.8**	**2.3**	**1.5**	**1.8**
Average (priority)		**2.2**			**1.8**			**1.7**	

Invertebrate BSAFs calculated from the model:

	TCDD			TetraCB			HpCDF		
BSAF - DEP	0.9	0.8	2.1	1.5	0.9	2.0	0.2	0.3	0.2
BSAF - FF	0.2	0.3	1.4	0.6	0.4	1.0	0.1	0.1	0.3
BSAF - DET	1.1	0.2	3.3	1.8	0.5	1.3	0.3	0.3	1.5
BSAF - C/O	0.8	0.3	2.6	1.5	0.5	1.5	0.1	0.2	0.7

EPA Alternate Calibrations – All SPAFs

EPA SPAF All

	2378-TCDD			TetraCB		
Species	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam
Phytoplankton						
Zooplankton						
Benthic invert deposit feeder		9.7	2.9		3.3	2.5
Benthic invert filter feeder						
Benthic invert detritivore						
Benthic invert carnivore/omnivore	5.6			3.5		
Small filter feeding fish		1.5			1.3	
Small forage fish	1.5	3.3	-1.7	-1.2	1.1	-1.1
Small American eel	-2.1	1.5	1.3	-2.2	1.1	1.2
Blue crab	-2.3	1.4	-13.7	-2.2	-1.0	-1.3
Carp		1.3	-1.6		-2.6	-1.1
Catfish	-2.1	2.8	-9.8	-2.6	1.2	-1.1
White perch	-1.7	1.3	-4.7	-2.1	-1.1	1.4
Large American eel	-1.3	1.2		-1.7	1.3	
Bass		1.1	-1.1		1.0	-2.0
Average (all)	**1.8**	**1.7**	**4.8**	**2.0**	**1.3**	**1.3**
Average (priority)	**1.8**			**1.5**		

EPA SPAF All – CFT model K_{ow}

	2378-TCDD			TetraCB		
Species	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam
Phytoplankton						
Zooplankton						
Benthic invert deposit feeder		23.9	7.2		2.0	1.5
Benthic invert filter feeder						
Benthic invert detritivore						
Benthic invert carnivore/omnivore	15.5			2.1		
Small filter feeding fish		1.8			-1.1	
Small forage fish	4.8	9.3	1.2	-2.2	-1.6	-1.7
Small American eel	1.1	2.9	2.4	-4.0	-1.6	-1.5
Blue crab	1.6	4.4	-4.8	-3.8	-1.8	-2.2
Carp		2.0	-1.2		-3.4	-1.4
Catfish	1.1	5.9	-5.3	-4.4	-1.4	-1.8
White perch	1.6	3.6	-2.2	-4.2	-2.1	-1.4
Large American eel	1.8	2.4		-3.0	-1.3	
Bass		3.0	1.9		-1.8	-3.8
Average (all)	**2.0**	**3.9**	**2.7**	**3.6**	**1.8**	**2.0**
Average (priority)	**3.7**			**2.3**		

EPA Alternate Calibrations – SPAF priority

EPA SPAF Priority

	2378-TCDD			TetraCB		
Species	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam
Phytoplankton						
Zooplankton						
Benthic invert deposit feeder		18.5	5.9		4.7	3.7
Benthic invert filter feeder						
Benthic invert detritivore						
Benthic invert carnivore/omnivore	9.2			4.5		
Small filter feeding fish		2.3			-1.1	
Small forage fish	-1.4	1.1	-9.1	1.2	1.1	-1.1
Small American eel	-2.1	1.2	-1.2	-1.7	-1.0	1.4
Blue crab	-1.5	1.4	-23.8	-1.4	1.2	-1.0
Carp		-1.0	-16.8		-1.1	1.2
Catfish	-3.9	-1.0	-33.5	-2.2	-1.0	-1.2
White perch	-1.1	1.3	-6.5	-1.5	-1.0	1.7
Large American eel	-1.3	-1.2		-1.6	-1.0	
Bass		-1.0	-2.9		1.4	-1.3
Average (all)	**1.9**	**1.3**	**13.4**	**1.6**	**1.1**	**1.3**
Average (priority)	**1.17**			**1.16**		

EPA SPAF Priority – CFT K_{OW}

	2378-TCDD			TetraCB		
Species	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam
Phytoplankton						
Zooplankton						
Benthic invert deposit feeder		17.3	5.5		2.4	1.8
Benthic invert filter feeder						
Benthic invert detritivore						
Benthic invert carnivore/omni	7.8			1.5		
Small filter feeding fish		2.2			-1.8	
Small forage fish	-1.5	-1.0	-9.4	-2.6	-2.3	-2.4
Small American eel	-2.3	1.1	-1.3	-4.9	-2.4	-1.8
Blue crab	-1.7	1.2	-26.6	-4.0	-2.1	-2.6
Carp		-1.0	-17.8		-1.9	-1.7
Catfish	-4.1	-1.0	-35.0	-6.0	-2.0	-2.6
White perch	-1.3	1.1	-7.1	-4.8	-3.1	-1.8
Large American eel	-1.4	-1.3		-4.1	-2.1	
Bass		-1.1	-3.2		-2.6	-4.7
Average (all)	**2.1**	**1.2**	**14.3**	**4.4**	**2.2**	**2.5**
Average (priority)	**1.2**			**2.7**		

EPA Alternate Calibration – Max Likelihood

EPA Max Likelihood

	2378-TCDD			TetraCB		
Species	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam
Phytoplankton						
Zooplankton						
Benthic invert deposit feeder		20.9	6.3		6.1	4.8
Benthic invert filter feeder						
Benthic invert detritivore						
Benthic invert carnivore/omnivore	7.9			5.4		
Small filter feeding fish		1.8			1.2	
Small forage fish	1.0	2.1	-4.5	1.4	1.4	-1.1
Small American eel	-2.0	1.6	1.1	-2.0	-1.1	-1.1
Blue crab	1.2	3.7	-6.4	-1.4	1.3	-1.1
Carp		-1.0	-10.9		-2.0	-1.9
Catfish	-2.6	1.8	-17.4	-2.6	-1.1	-1.8
White perch	-1.2	1.8	-4.3	-1.5	1.2	1.4
Large American eel	-1.4	1.0		-1.7	1.0	
Bass		-1.2	-2.9		-1.1	-3.1
Average (all)	**1.6**	**1.8**	**6.8**	**1.8**	**1.3**	**1.6**
Average (priority)	**1.7**			**1.3**		

EPA Max Likelihood – CFT K_{OW}

	2378-TCDD			TetraCB		
Species	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam
Phytoplankton						
Zooplankton						
Benthic invert deposit feeder		21.7	6.6		2.1	1.6
Benthic invert filter feeder						
Benthic invert detritivore						
Benthic invert carnivore/omnivore	8.3			1.5		
Small filter feeding fish		1.8			-1.6	
Small forage fish	1.1	2.2	-4.4	-2.7	-2.2	-2.4
Small American eel	-1.9	1.7	1.2	-6.4	-2.9	-2.6
Blue crab	1.2	3.8	-6.1	-4.6	-2.1	-2.9
Carp		-1.0	-10.7		-3.0	-3.0
Catfish	-2.5	1.9	-17.1	-7.6	-2.4	-3.7
White perch	-1.2	1.9	-4.2	-6.0	-3.3	-2.3
Large American eel	-1.4	1.1		-5.2	-2.5	
Bass		-1.2	-2.8		-3.8	-8.5
Average (all)	**1.5**	**1.8**	**6.6**	**5.4**	**2.6**	**3.6**
Average (priority)	**1.7**			**3.3**		

Review of EPA Alternate Calibrations

- Takeaways
  - Calibration of K_{ow} is driving model performance improvements
  - Benthic E_D – potential to improve model performance, would need to calibrate model with this additional parameter
  - Parameter value substitutions – model performance did not improve, not surprising since values were calibrated along with K_{ow}

Review of EPA Alternate Calibrations

- Suggestions
  - Re-run 3 calibrations with following conditions:
    - With matching distributions (CPG to provide) without K_{ow} held constant
    - With matching distributions (CPG to provide) with K_{ow} held constant
  - Compare parameter values from those scenarios with current parameter values.
  - Incorporate benthic E_D?
    - Fundamentals of modeling – don't add additional parameters for small improvements in model fit

Key Uncertainties

- K_{OW} and E_D (but improved understanding based on literature review)
- Characterization of benthic invertebrate community (high variability)
- Fish ages and growth rates
- Fish diets (high variability)

Next Steps

- Finalize current model calibration
  - What is needed to achieve this?
  - Caveat that model will be re-evaluated after collection of current condition samples.
- Update alternate calibrations
- Prepare model documentation
  - Model sensitivity/uncertainty based on various analyses done to date.
  - Model updates specific to Passaic model